ARKIV FÖR FYSIK Band 11 nr 20

Read 6 June 1956

On the connection between electrical resistivity and potential energy in pure metals

By G. Borelius

With 2 figures in the text

Recent studies [1, 2] of the thermal agitation in crystals from the point of view of density fluctuations revealed an intimate connection between the potential part of the thermal energy and the change of volume with change of temperature or at fusion. The cause for this connection is that in pure metals the potential energy and the thermal expansion are both dependent on the disorder of the lattice caused by thermal agitation. Now the electrical resistivity of pure metals is also generally assumed to depend on lattice disorder and it is near at hand to look for a connection between the resistivity on one side and the potential energy or the thermal expansion on the other. We shall here compare resistivity and potential energy for eight cubic metals for which suitable data have been found in the literature.

As an approximate measure of the potential energy U pro mole at a temperature of T°K we take as in earlier papers [2, 3]

$$U = \int_0^T C\,dT - \frac{3}{2} R\,T\,D\left(\frac{T}{\theta}\right), \tag{1}$$

i. e. the difference between the total energy obtained by integration over the molar heat C at constant (practically zero) pressure and the kinetic energy obtained as the product of the classical value 3RT/2 and the Debye function

$$D\left(\frac{T}{\theta}\right) = 3\left(\frac{T}{\theta}\right)^3 \int_0^{\frac{\theta}{T}} \frac{x^3}{e^x - 1}\,dx \tag{2}$$

which goes from 0 to 1 for increasing T/θ, θ being the Debye characteristic temperature.

In Figs. 1 and 2 we have plotted the relative resistances r/r_0, r_0 being the resistance at 0°C, against the potential energy U.

Fig. 1 shows these plots for the five face-centerad cubic metals Al, Cu, Ag, Au, and Pb arranged in order of decreasing characteristic temperatures θ, obtained from specific heat data at low temperatures and given in the table. Fig. 2 shows the

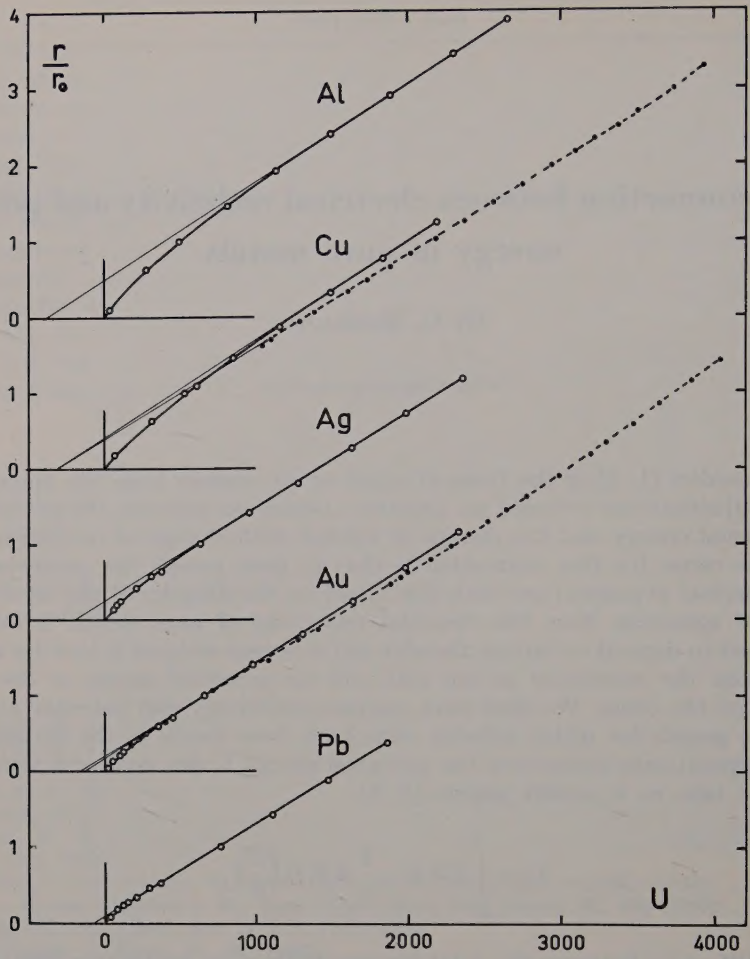

Fig. 1. Reduced resistance versus potential energy in cal/mole for face-centered cubic metals.

plots for the body-centered cubic metals Li, Na, and W. The sources for the calculation of the potential energy U are acounted for in earlier papers [2, 3]. The resistivity data are obtained from the papers refered to in the table. For W the data are obtained from a published diagram.

From the zero points of the diagrams, corresponding to 0°K, the curves seem to start approximately linearly. Exact linearity would mean proportionality between resistance and the potential energy U, which at low temperatures is half of the total energy and thus approximately proportional to the fourth power of the absolute temperature T. The resistance, too, would thus be proportional to T^4. According to current theories the resistance is assumed to vary as T^5. From an experimental point of view, it is still not possible to choose between T^4 and T^5.

In a range corresponding to about $0.3 < T/\theta < 1.5$ the curves bend and continue

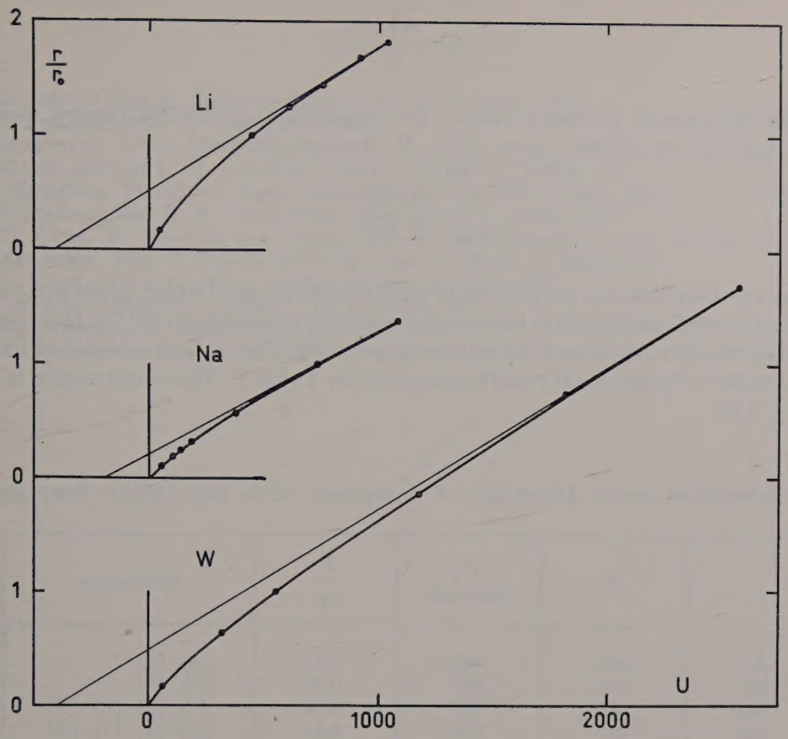

Fig. 2. Reduced resistance versus potential energy in cal/mole for body-centered cubic metals.

as straight lines with a slope that is about half the initial slope. Extensions of the straight parts cut the energy axis at points corresponding to negative values, U_z. In some cases, Cu and Au, there is a slight bending upwards of the curves when the temperatures approach the melting point. We have here obtained U_z from the inflexion tangent which contacts the curve over a wide range. For Pt and Mo, the experimental curves are bending downwards at high temperatures, and it is difficult to know how to draw the extension line. As for the present we are mainly interested in the extensions, we have excluded these metals from our discussion.

The linear parts of the curves in the range $T > 1.5\ \theta$ can thus be described by the equation

$$r = \text{const.} \times (U + U_z). \tag{3}$$

It appears from the figures that U_z increases with increasing characteristic temperature, and from the experimental point of view, it is in fact possible to interpret the U_z as the potential halves of the zero-point energies. In this case we should have

$$U_z = \frac{3}{2} N \frac{h\bar{\nu}}{2}, \tag{4}$$

where N is the number of atoms pro mole, h the Planck constant, and $\bar{\nu}$ the mean value of the lattice frequencies at the sero point. For the Debye characteristic temperature we have

$$\theta = \frac{h\nu_D}{k}, \tag{5}$$

k being the Boltzmann konstant and ν_D the upper limit of the frequency spectrum. From (4) and (5) we obtain, since $Nk = R$, the gas constant,

$$\frac{\bar{\nu}}{\nu_D} = \frac{4}{3}\frac{U_z}{R\,\theta}. \tag{6}$$

The frequency distribution, proportional to ν^2, assumed by Debye, gives $\bar{\nu}/\nu_D = 0.75$. From a complicated distribution function obtained by Leighton [12] for face-centered cubic crystals we have deduced the value $\bar{\nu}/\nu_D \doteq 0.68$. The values calculated by equation (6) from the experimental results are given in Table 1. The uncertainty is of the order of ± 0.10.

Table 1. Calculated mean frequency $\bar{\nu}$ compared with the Debye frequency ν_D.

	θ	U_z cal/mole	$\frac{\bar{\nu}}{\nu_D}$	References
Al	398	390	0.66	[4], [5]
Cu	325	280	0.58	[5], [6]
Ag	215	190	0.59	[5], [7], [8]
Au	190	170	0.60	[5], [6], [7], [8]
Pb	88	75	0.57	[5], [7], [8]
Li	363	400	0.74	[9], [10]
Na	159	190	0.80	[9], [10]
W	310	390	0.84	[5), [11]

These experimental values for $\bar{\nu}/\nu_D$ are consistent with the interpretation of U_z as the potential half of the zero-point energy. We are thus led to the conclusion that the zero-point energy, which at zero temperature gives no contribution to the resistivity, at higher temperatures cooperates with the thermal potential energy to maintain the lattice disturbances causing the resistivity.

For the face-centred cubic metals the thermal increase in volume as a function of the potential energy is found [2] to give a curve that continues from the solid to the liquid state.. We have looked for a similar continuity of the resistivity as a function of the potential energy. Unfortunately the available results of resistivity measurements on liquid metals are widely diverging and neither approve nor disapprove the existence of a continuity.

The author is indebted to Mr. L. E. Larsson for help with the numerical work.

Stockholm, Physics Department, Royal Institute of Technology.

REFERENCES

1. G. Borelius and A. Sandin, Arkiv f. Fysik *10* (1955), 187.
2. G. Borelius, Arkiv f. Fysik, in press.
3. G. Borelius, Arkiv f. Fysik, in press.
4. G. Borelius and L. E. Larsson, Arkiv f. Fysik *11* (1956), 137.
5. W. Meissner, Handb. d. Experimentalphysik, Bd XI:2 (1935), 53.
6. C. J. Mechan and R. R. Eggleston, Acta Metal. *2* (1954), 680.
7. P. G. Cath, H. Kamerlingh Onnes, and J. M. Burgers, Comm. Leiden nr *152* (1918).
8. L. Holborn, Ann. d. Physik *59* (1919), 145. Z. Physik *8* (1921), 58.
9. D. K. C. MacDonald, Prop. in Met. Physics *3* (1952), 62.
10. A. Bernini, Phys. ZS *5* (1904), 241; *6* (1905), 74.
11. E. Nachtigall, Z. Metallkunde *43* (1952), 23.
12. R. B. Leighton, Rev. Mod. Physics *20* (1948), 165.

Tryckt den 5 november 1956

Uppsala 1956. Almqvist & Wiksells Boktryckeri AB